CHE 3G04 – CHEMICAL PROCESS SYNTHESIS AND SIMULATION

COURSE OUTLINE 2024

COURSE DETAILS

Instructor: Dr. Giancarlo Dalle Ave
dalleagf@mcmaster.ca

Teaching Assistants:
Enrique Luna Villagomez lunavile
Barnabas Osei oseib2
Nagat Elrefaei elrefaen

Lectures:
Mo, Thu 09:30, Tu 10:30 - PC 155

Tutorials:
Mo 10:30-12:30 - BSB 244
Wed 14:30-16:30 - BSB 241
Thu 12:30-14:30 - KTH B121

Office Hours:
Instructor: Mo 15:30-17:30 JHE 345/B
Additional office hours by appointment
TAs: By appointment only

Prerequisites: ChE 2E04, ChE 2F04, ChE 3A04, ChE 3D04, ChE 3M04

McMaster University

DESCRIPTION

Chemical process design and simulation including models for heat exchangers, separators, reactors, heat integration, pressure handling, energy conversion, and other unit operations. Using process simulations to solve problems related to chemical processing, energy, and sustainability.

LEARNING OUTCOMES

Students who complete this course should be able to use chemical process flowsheet simulations to solve problems in the chemical industry. This includes:

- L1: Starting with a chemical or business objective (e.g., create so much of product A from raw materials B), synthesize a flowsheet on paper which could achieve this objective.
- L2: Implement this flowsheet in a simulation program such as Aspen Plus.
- L3: Make use of thermophysical property models in the flowsheet. This includes identifying the correct models to use.
- L4: Make use of unit operation models which are built in to the software for common units such as heat exchangers, distillation columns, pumps, compressors, reactors, and mixers.
- L5: Construct custom models for unit operations which are not built into the software, and integrate them into the flowsheet.
- L6: Successfully run the flowsheet simulation to compute all mass and energy balances.
- L7: Extract useful information from the results and apply it towards the solving of the original problem.

▪L8: Perform advanced functions such as sensitivity analyses, case studies, or optimization to re-use the flowsheet thousands of times over and get an incredible amount of useful data.

▪L9: Use the results of these flowsheet simulations to compute capital costs, energy costs, operation costs, and emissions to the environment.

▪L10: Use these cost and impact results to make an assessment of the sustainability of the process using the triple-bottom-line of sustainability approach.

COURSE STRUCTURE

COURSE BOOKS

1) Seider, *et. al*. "Product & Process Design Principles", 4th Edition, ISBN: 978-1-119-28263-1 (3rd edition works as well)
2) Adams II. "Learn Aspen Plus in 24 Hours", 2nd edition, ISBN: 9781264266654 (1st edition also works), Available online here (may have to access via university library website): https://www.accessengineeringlibrary.com/content/book/9781264266654

LECTURES

▪Lectures will be delivered live from PC 155. Lectures will be recorded and posted online within 48 hours after the lecture (unless something goes wrong with the recording which happened before). Lectures will be posted to the course YouTube Playlist.

▪Tutorials will be live in the computer lab and **attendance is required for marks** (in-tutorial assignments).

IF THE INSTRUCTOR CANNOT ATTEND

Due to my ongoing family situation I may miss a class once in a while. If so, a recorded version of the lecture will be posted online to the YouTube playlist instead.

COURSE POLICIES

GRADING POLICIES

Valid MSAF forms for missed written midterms, labs, or assignments will result in weight transferring to the final. MSAFs for the in-lab midterm will result in a retake.

Midterm and final exams will be open book, open note, and open device. All devices must be in airplane mode. If you're found to have a device not in airplane mode, you will automatically be given a zero on the exam. Any calculator may be used during the exams.

If technical difficulties prevent digital submissions to A2L, email it to a TA/the instructor instead before the submission deadline.

CURVING POLICY

Only final grades will be curved based on the instructor's discretion. The curve will never lower your grade, it can only improve it or leave it unchanged.

ACADEMIC DISHONESTY

All marked exams are to be done individually, with no collaboration with anyone. Collaboration is encouraged for assignments which can be completed in groups of up to three.

Tutorials will not be marked other than for completion. Feel free to work in groups. It is for your understanding. If you work better alone, do it alone.

Plagiarism, improper collaboration, copying unauthorized tests or aids, and other academic dishonesty will not be tolerated. Your first offence will be reported to the Office of Academic Integrity.

The default penalty for academic dishonesty is a zero on the entire exam / quiz / project, even if the dishonesty occurred on just one portion or question of that exam / quiz / project. However, if Academic Integrity chooses to hold a hearing, they determine the penalty which replaces the default penalty.

Note: You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity. Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: "Grade of F assigned for academic dishonesty"), and/or suspension or expulsion from the university.

It is your responsibility to understand academic dishonesty. See the Academic Integrity Policy at http://mcmaster.ca/academicintegrity

GRADING BREAKDOWN

	Weight	Comment	Proposed Due Dates
Tutorials	10%	10 tutorials (completion marks) Note there are 11 tutorials scheduled meaning you can skip 1 and still get full marks or attend all 11 for a bonus mark.	Weekly
Assignments	10%	Two assignments (one before the written midterm and one before the exam period (5% each)	1: Feb 13th 2: Apr 4th
Midterms	30%	15% written + 15% Aspen midterms. More details on later pages.	Written: Week of Feb 26th Aspen: Week of Apr 1st
Project	20%	Includes graded milestone deliverables throughout the term. More details on later pages.	1: Jan 29th 2: Mar 4th[t] 3: March 21st Final Presentations: Week of April 8th
Final Exam	30%	2.5 hour written exam	TBD

COURSE NOTES

Note that all above due dates as well as the breakdown are subject to change. It is unlikely that major changes will occur but be sure to check on Avenue for minor changes to the grade breakdown and the due dates.

TERM PROJECT

Term projects will be completed in groups of four or five. The project will be comprehensive and include everything learned in the course. You will complete the project in stages over the course of the term by meeting the required project milestones (which will be graded mainly for feedback purposes).

You will be permitted to choose your own groups. If you are not part of a group, I will assign you to a group. I may have to assign you to a group that has already formed. I have executive power to reassign and reform any group as I please, but I will only do this if the system is abused or if extreme circumstances warrant. I highly recommend you chose groups from within your tutorials so you can meet together during tutorial times.

The term projects will be partially delivered in the form of a presentation/oral examination with supporting materials such as simulation code, spreadsheets, calculations, and written deliverables. Points will be awarded for both technical accuracy as well as quality of the communication. Portions of the project will be delivered as milestones during the term. The purpose of the milestones will be to give you feedback on the project progress so that you have time to reevaluate design/simulation decisions going forward.

The project will be related to synthesizing and analyzing a flowsheet which can be used to solve some chemical engineering problem. The results will be analyzed with regards to the triple-bottom-line of sustainability: cost, social impact, and environmental impact.

TERM PROJECT GRADING

Milestones Portion 20%

Four milestone deliverables, worth 5% of the project each (1% overall grade). Think of these as homework. The proposed due dates for the project deliverables are:

- Milestone 1: Process Design – Jan 29th 2024

▪Milestone 2: Process Simulation – Mar 4th 2024

▪Milestone 3: Process Optimization - Mar 21st 2024

▪Milestone 4: Economics + sustainability assessment: Apr 8th 2024

Presentation/Oral Exam, Group Portion 60%

The final project deliverable is a group presentation presenting key design and simulation decisions as well as a summary of results. The presentations will occur the week of April 8th. An oral exam will follow in which groups must defend their submission and the decisions they made. Note that no design is ever perfect, part of the oral exam will focus on your ability to recognize things that could have been done better and discuss how you could go about changing them.

Presentation/Oral Exam, Individual Portion 20%

At the oral defence, you will be asked individual questions for individual credit. The instructor reserves the right to adjust the weight of the group and individual components of the oral exams per individual at any time.

COURSE SOFTWARE

In this course, you will learn how to use chemical engineering software commonly used throughout the industry today. This will include:

▪**Aspen Plus**: A sequential-modular flowsheeting simulation program (EOR methods not covered) popular in the chemical and petrochemical industry. You are not required to purchase this software (you can't afford it!). It is available in all the UTS labs for free.

▪**Aspen Capital Cost Estimator**: A program which computes very detailed capital cost estimates for chemical process equipment. Also available in the UTS Labs.

▪**Aspen Energy Analyzer**: A program which creates an optimized heat exchanger network for your process. You will use this in the UTS Labs.

MIDTERMS

The course will consist of two midterms. One written midterm and one in-lab midterm.

The written midterm will take place the evening of February 28th.

The Aspen midterm will be a timed takehome midterm where you will be required to simulate a flowsheet in Aspen Plus. The midterm must be completed individually. The midterm will take place the week of Apr. 1st, no tutorials will take place this week. The normal tutorial time can be used to complete the mideterm.

COURSE CALENDAR

The course is broken down into four major units:

▪Unit 1: Process Flowsheeting: Reading, drawing, and understanding process flowsheets. We will also look at synthesising new flowsheets, handling steady states, recycles, escape routes, pressure-driven flows, and other key fundamentals.

▪Unit 2: Chemical Process Simulators: Common models and heuristics. Choosing the right models. Mathematical principles for solving systems of equations. DOF for physical properties and flowsheets. Sequential modular programs. Recycle, tears, and equation-of-state solvers.

▪Unit 3: Unit Operation Modeling: Equilibrium, Gibbs, extent of reaction, and kinetic reactor models. Flash drums, distillation, stripping, and rectification. Equilibrium and rate-based distillation.

▪Unit 4: Triple Bottom Line of Sustainability: Using software for equipment costing and economics. Operating costs, utilities, feed costs, raw materials, labour, and energy costs. Life cycle analyses, society impacts, responsibilities. Using software to determine the sustainability of chemical processes and supply chains.

An approximate course calendar can be found in the table on the next page (which subject to change depending on how fast I talk in class).

ASSIGNMENTS

The course will have two assignments each worth 5% of the overall grade. The assignments can be completed in groups of up to three (maximum three) people. The assignments are meant to provide practice for the written midterm/exam.

Week	*Date*	*Unit*	*Lecture Topic*	*Tutorial*	*Assigned*	*Due*	*Book Chapters*
1	08-01-2024	1-1	Intro	1 - Getting started with Aspen Plus			Ch 2 (4)
	09-01-2024	1-2	Design Principles		Project pt. 1 Project team survey		
	11-01-2024	1-3	Design and Pressure				
2	15-01-2024	1-4	Temperature management	2 – Physical Property Modeling		Project team survey	Ch 6.5-6.7, 12.2 (18.2), 14 (20)
	16-01-2024	1-5	Recycles, purges, waste				
	18-01-2024	1-6	Separation heuristics				
3	22-01-2024	1	Review	3 – Problem Solving Tools			Ch 6-6.4, 6.8-6.10, 9 (8)
	23-01-2024	1-7	Conceptual design workshop				
	25-01-2024	2-1	Thermophysical property models				
4	29-01-2024	2-2	EoS models	4 – Heat Exchangers	Project pt. 2	Project pt. 1	Ch 12.2 (18.2)
	30-01-2024	2-3	Phase equilibria				
	01-02-2024	2-4	Flash calculation + DoF				
5	05-02-2024	2-5	Activity coefficient models	5 – Equilibrium-Based Distillation Models	Assignment 1		
	06-02-2024	2-6	HeatX and Split Models				
	08-02-2024	2-7	Sequential Modular Flowsheeting				
6	12-02-2024	2	Review	6 – Advanced Problem Solving Skills			
	13-02-2024	1+2	Written Midterm Review			Assignment 1	
	15-02-2024	1+2	Assignment 1 Review				
7	26-02-2024	3-1	Rstoic and Ryield	7 – Chemical Reactor Models	Project pt. 3	Written midterm on Feb 28th	Ch 7 (5), 15.2 (N/A)
	27-02-2024	3-2	Equilibrium models				
	29-02-2024	3-3	Kinetic Reaction Models				
8	04-03-2024	3-4	HeatX Networks	9 – Custom Models + External Control		Project pt. 2	Ch 11-11.4 (9-9.4)
	05-03-2024	3-5	Shortcut distillation models				
	07-03-2024	3-6	Equilibrium distillation models				
9	11-03-2024	3	Review	11 – Heat Exchanger Networks			Ch 13-13.5 (19-19.5
	12-03-2024	1+2	Written midterm take up				
	14-03-2024	4-1	Intro to sustainability				
10	18-03-2024	4-2	Costs and economics	8 -Rate-Based Distillation	Project pt. 4		Ch 3.3-3.5 (N/A) 16 (22)
	19-03-2024	4-2	Capital Costs				
	21-03-2024	4-3	Operating Costs			Project pt. 3	
11	25-03-2024	4-4	LCA Boundaries	10 – Capital Cost Estimation	Assignment 2		
	26-03-2024	4-5	LCI				
	28-03-2024	4-6	LCIA				
12	01-04-2024	4-7	Social Impacts	Aspen Midterm Week			
	02-04-2024	4	Review				
	04-04-2024	All	Exam Review				
13	08-04-2024	3+4	Assignment 2 Review			Assignment 2	
	09-04-2024					Project Presentations	

TUTORIALS

Tutorials in this class will be in-lab where you will gain first hand experience of the software in the course. These tutorials will be marked for completion (they have to be correct to get the full marks). The tutorial instructions are very detailed so following them directly should enable you to easily complete the tutorials.

We will be covering the tutorials in a different order than the textbook. The TAs are aware of this, but please ensure you complete the right tutorial in any given week. To avoid any confusion, the tutorial activities are also presented in the approximate course calendar given above. The number in the table corresponds to the "Tutorial Activity Number" in the second edition textbook. Please make sure to complete the correct tutorial for each week.

IMPORTANT LINKS

Please find below a list of important links for the class. They'll be mentioned throughout the term but a comprehensive list follows:

YouTube Lecture Playlist

Project Group Formation Survey

Feedback Form

Instructor/TA Emails:

Giancarlo Dalle Ave: dalleagf@mcmaster.ca
Enrique Luna Villagomez: lunavile@mcmaster/ca
Barnabas Osei: oseib2@mcmaster.ca
Nagat Elrefaei: elrefaen@mcmaster.ca

OTHER/MISC.

THE P.R.O.C.E.S.S.

The department of Chemical Engineering has a storied history of education. In addition to teaching and learning, the department is proud of our graduates not only for their academic success, but their more intrinsic traits that make them respected members of the engineering community.

Recently, several high-ranking graduates from the McMaster Chemical Engineering Program employed in various industries (oil/gas, financials, etc.) were interviewed to ask what traits they look for when hiring for engineering positions. Using this information, the department would like to present to you the PROCESS: a code of conduct that we hope will guide our students throughout this program and their careers to come.

- **P**rofessionalism
- **R**esponsibility
- **O**wnership
- **C**uriosity
- **E**mpathy
- **S**elflessness
- **S**ervice

It is up to YOU to interpret these traits and apply them to your time at McMaster and your career as you see fit. These traits will not be assessed for grades but will be strongly encouraged throughout your time at McMaster. We hope that you identify with these character traits and what they mean to you, and that you trust the process.

INCLUSIVE ENVIRONMENT

Everyone in our teaching team considers the classroom to be a place where you will be treated with respect, and we welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability – and other visible and non-visible differences. All members of the class are expected to contribute to a respectful, welcoming, and inclusive environment for every other member of the class. We will gladly honour your request to address you by an alternate name or gender pronoun. Please advise us of this preference early in the semester.

COPYRIGHT AND RECORDINGS

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, including lectures by University instructors.

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by a student for the purpose of personal study. If you actually read this, please send the instructor your favourite gif of a cute animal for a small bonus to your final grade. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

ACADEMIC ACCOMMODATIONS FOR RELIGIOUS, INDIGENOUS, OR SPIRITUAL OBSERVANCES

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the RISO policy. Students should submit their request to their Faculty Office normally within 10 working days of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

C.E.A.B. GRADUATE ATTRIBUTES

Certain courses in the chemical engineering curriculum collect indicator data related to the development of the attributes deemed critical for engineers according to the Canadian Engineering Accreditation Board (CEAB). These indicators (detailed at the beginning of the outline) will be assessed throughout the course and redacted samples of student work may be collected for submission to the CEAB during McMaster Engineering's accreditation cycle. The indicators assessed in ChE 3G04 are as follows:

1.4 – Competence in mathematics.

4.3 – Competence in engineering fundamentals.

4.4 – Evaluates engineering tools, identifies their limitations, and selects, adapts, or extends them appropriately.

5.2 – Successfully uses engineering tools.

9.1 – Demonstrates comprehension of technical and non-technical instructions and questions.

11.1 – Applies economic principles in decision making

The CEAB indicators listed above are mapped to the course learning outcomes as shown in the following table. The CEAB accreditation process is an important component to curriculum design in engineering. If you have any questions or wish to be involved in the accreditation process, please let me know at dalleagf@mcmaster.ca.

Indicator	Mapped Learning Outcomes
1.4	L1, L3, L4
4.3	L2, L4, L5
4.4	L7
5.2	L5, L6, L8
9.1	L 9, L10
11.1	L9, L10